

Wavefront solution in extended quantum circuits with charge discreteness

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A wavefront solution for quantum (capacitively coupled) transmission lines with charge discreteness (PRB **64**, 235309 (2001)) is proposed for the first time. The nonlinearity of the system becomes deeply related to charge discreteness. The wavefront velocity is found to depend on a step discontinuity on the (pseudo) flux variable, f , displaying allowed and forbidden regions (gaps), as a function of f . A preliminary study of the stability of the solutions is presented. The dual transmission line hamiltonian is proposed and finally, we find a connection with the (quantum) Toda lattice.

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I. INTRODUCTION

Today, the broad field of nanostructure is at the heart of many technological devices^{1,2,3,4,5}. Naturally, at this scale and for low temperature, quantum mechanics plays a fundamental role⁴. Recently, much effort has been devoted to study nanostructures, using as model that of quantum circuits with charge discreteness^{6,7,8,9,10,11,12}. Work has been published on subjects such as persistent currents^{6,7}, coupled quantum circuits^{8,9}, the electronic resonator¹⁰, quantum point contacts¹¹, and others². In this article, we are interested in spatially extended quantum circuits (transmission lines) with charge discreteness. This is an interesting specific theoretical subject of broad potential applications, since nano-devices could be put together forming chains, and then be viewed as electric transmission lines. For instance, electric transport properties in DNA have been measured recently^{13,14,15}; some degree of disagreement related to conducting properties exists, nevertheless, it is clear that the DNA molecule could be viewed and modeled as a quantum transmission line. Moreover, molecular electronic circuits¹⁶ are actively studied theoretically and experimentally. In such systems, chains of individual molecules form a line of circuits. Therefore, quantum circuits is a broad field involving future applications from the perspective of nano-devices, electric transmission in macromolecules, left-handed materials, Toda lattice, and others.

In this work we will consider a wavefront solution for an extended quantum circuit (transmission line). For the first time, a sequence of bands and gaps is found and characterized for this specific system with charge discreteness, giving hopes for the description of more complex extended systems (dual transmission lines, complex basis, etc.).

In section II we will introduce the Hamiltonian for coupled circuits, and the equations of motion for the spatially continuous systems. In Sec. III, the wavefront

solution is obtained and the band-gap structure is characterized, in Sec. IV the stability question is considered. In Sec. V the dual line hamiltonian is introduced. In Sec. VI the connection with Toda lattice is presented. Finally, we state our conclusions.

II. QUANTUM TRANSMISSION LINES WITH DISCRETE CHARGE

It is known that for a chain of quantum capacitively-coupled quantum circuits with charge discreteness (q_e), the Hamiltonian may be written as⁸:

$$\hat{H} = \sum_{l=-\infty}^{\infty} \left\{ \frac{2\hbar^2}{Lq_e^2} \sin^2\left(\frac{q_e}{2\hbar}\hat{\phi}_l\right) + \frac{1}{2C} \left(\hat{Q}_l - \hat{Q}_{l-1}\right)^2 \right\}, \quad (1)$$

where the index l describes the cell (circuit) at position l , containing an inductance L and capacitance C . The conjugate operators, charge \hat{Q} and pseudoflux $\hat{\phi}$, satisfy the usual commutation rule $[\hat{Q}_l, \hat{\phi}_{l'}] = i\hbar\delta_{l,l'}$. A spatially extended solution of Eq. (1) will be called a *cirquiton like solution*, corresponding to the quantization of the classical electric transmission line with discrete charge (i.e. elementary charge q_e). Note that in the formal limit $q_e \rightarrow 0$ the above Hamiltonian gives the well-known dynamics related to the one-band quantum transmission line, similar to the phonon case. The system described by Eq. (1) is very cumbersome since the equations of motion for the operators are highly nonlinear due to charge discreteness. However, this system is invariant under the transformation $Q_l \rightarrow (Q_l + \alpha)$, that is, the total pseudoflux operator $\hat{\Phi} = \sum \hat{\phi}_l$ commutes with the Hamiltonian; in turn, the use of this symmetry helps us in simplifying the study of this system.

To handle the above Hamiltonian, we will assume a continuous approximation (infrared limit); that is to say,

we shall use $(Q_l - Q_{l-1}) \approx \partial Q / \partial x^{17}$. In this way, it is possible to re-write the sum of Eq. (1) as the integral $\sum_{l=-\infty}^{\infty} \approx \int_{-\infty}^{\infty} dx$, where x is a dimensionless variable used to denote the position in the chain (i.e. the equivalent of l), since we have not introduced so far the cell size of the circuit. In this approximation, the Hamiltonian becomes

$$\hat{H} = \int_{-\infty}^{\infty} \hat{\mathcal{H}} dx = \int_{-\infty}^{\infty} \left\{ \frac{2\hbar^2}{Lq_e^2} \sin^2\left(\frac{q_e}{2\hbar}\hat{\phi}\right) + \frac{1}{2C} \left(\frac{\partial \hat{Q}}{\partial x}\right)^2 \right\} dx, \quad (2)$$

where $\hat{\mathcal{H}}$ represents the Hamiltonian density operator for the fields $\hat{\phi}(x)$ and $\hat{Q}(x)$ and where $[\hat{Q}(x), \hat{\phi}(x')] = i\hbar\delta_{x,x'}$. From the above Hamiltonian we find the equations of motion (Heisenberg equations):

$$\frac{\partial}{\partial t} \hat{\phi} = \frac{1}{C} \frac{\partial^2}{\partial x^2} \hat{Q}, \quad (3)$$

$$\frac{\partial}{\partial t} \hat{Q} = \frac{\hbar}{Lq_e} \sin\left(\frac{q_e}{\hbar}\hat{\phi}\right). \quad (4)$$

III. WAVEFRONT SOLUTIONS

As stated previously, we are interested in wavefront-like solutions of the system of Eqs.(3-4). We proceed in the standard way¹⁷, by assuming travelling wave solutions for our operators, i.e., we define a new variable $z = x - vt$, and assume

$$\hat{Q}(x, t) = \hat{Q}(z), \quad (5)$$

$$\hat{\phi}(x, t) = \hat{\phi}(z), \quad (6)$$

where v stands for the unknown propagation velocity with dimensions of inverse time, since we did not introduce a grid length parameter in our continuum approximation. Therefore, from the Heisenberg equations of motion (3-4), the wavefront equations in the new variable z become

$$-v \frac{d}{dz} \hat{\phi} = \frac{1}{C} \frac{d^2}{dz^2} \hat{Q}, \quad (7)$$

$$-v \frac{d}{dz} \hat{Q} = \frac{\hbar}{Lq_e} \sin \frac{q_e}{\hbar} \hat{\phi}. \quad (8)$$

From the above pair of equations we obtain a closed equation for the pseudoflux operator resulting in the "eigenvalue" problem:

$$\frac{\hbar}{LCq_e} \sin \frac{q_e}{\hbar} \hat{\phi}(z) = v^2 \hat{\phi}(z), \quad (9)$$

where the integration constant has been chosen as zero by simplicity (however, see eq. 14). Equation (9) corresponds to an eigenvalue problem for the non-linear super-operator $\mathcal{L}(\hat{\phi}) = \sin(\hat{\phi})$. There is at least two kinds

of solutions: a projection operator $\hat{\phi} = \hat{P}$, satisfying $\hat{P}^2 = \hat{P}$, and $\hat{\phi} = \hat{\sigma}$ satisfying $\hat{\sigma}^2 = 1$. For simplicity, we shall consider only the first case (a projector). Consider the pseudoflux operator only in one LC-cell of the chain, and its spectral decomposition in the Schrödinger picture $\hat{\phi}_{cell} = \int \phi |\phi\rangle \langle \phi| d\phi$. Now, pick-up only one term from there (call it ϕ_0 , say) and consider now the well-defined operator

$$\hat{\phi} = f \hat{P}_0 \quad \text{where} \quad \hat{P}_0 = |\phi_0\rangle \langle \phi_0|, \quad (10)$$

where f is an arbitrary pseudoflux parameter, and replace into Eq.(9). At this point, a note concerning the validity for the commutation rules may be in order: the projector operator \hat{P}_0 defines a one dimensional subspace in which subspace the commutation rule between $\hat{\phi} = f \hat{P}_0$ and the projected charge operator $\hat{P}_0 \hat{Q} \hat{P}_0$, is verified.

Now, since \hat{P}_0 is a projector, then the equation for the pseudoflux f becomes related to the velocity by

$$v^2 = \frac{1}{LC} \frac{\sin(q_e f / \hbar)}{(q_e f / \hbar)}. \quad (11)$$

Since both signs $(\pm f)$ are possible, then we can construct the wavefront solution (step 2f) of the equations of motion (3-4):

$$\hat{\phi}_{sol}(z) = \begin{cases} +f \hat{P}_0, & z > 0 \\ -f \hat{P}_0, & z < 0 \end{cases}, \quad (12)$$

corresponding to a solution with zero total flux (Sec. I). Concerning the matching condition at $z = 0$, the solution (12) is in complete agreement with the matching implying explicitly Eqs.(7-8).

The condition $v^2 \geq 0$ on the wave-front velocity gives the band-gap conditions on the system. In fact, from (11) the restriction

$$\frac{\sin \frac{q_e}{\hbar} f}{\frac{q_e}{\hbar} f} \geq 0, \quad (13)$$

means that there exists a sequence of bands and gaps. The figure 1 shows a plot of the wavefront velocity (11) for different values of the pseudoflux f , in which it is seen an alternating sequence of bands and gaps, corresponding to propagating and forbidden modes. Note that the main allowed band $(-\pi\hbar/q_e < f < \pi\hbar/q_e)$ is twice as wide as the other allowed bands.

Recall that the integration constant was set equal to zero to obtain (9), now consider the nonzero case, then the wavefront velocity becomes formally

$$v^2 (\hat{\phi} - \hat{C}) = \frac{\hbar}{LCq_e} \left(\sin \frac{q_e}{\hbar} \hat{\phi} - \sin \frac{q_e}{\hbar} \hat{C} \right). \quad (14)$$

where \hat{C} is an integration constant.

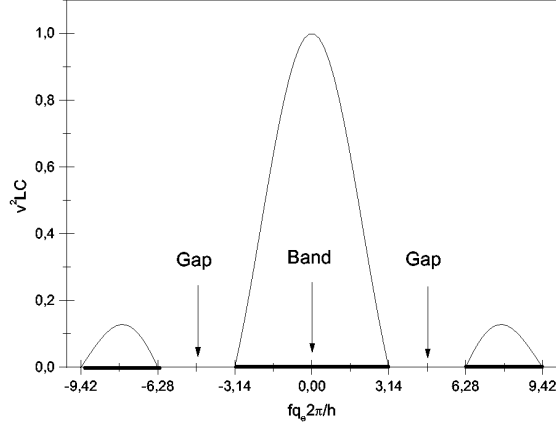


FIG. 1: Plot of the velocity of the wavefront, as a function of the flux parameter f . As specified by Eq. (11) there is a structure of bands and gaps. The main allowed velocity band is twice as wide as the other allowed bands. This structure is a direct consequence of charge discreteness, an effect that disappears in the limit $q_e \rightarrow 0$.

IV. STABILITY

We present some preliminary results concerning the stability of the solution (10); a more detailed treatment is currently under consideration. Consider now the perturbative solutions

$$\begin{aligned}\hat{\phi} &= \hat{\phi}_{sol} + \hat{\varepsilon} \\ \hat{Q} &= \hat{Q}_{sol} + \hat{\eta},\end{aligned}\quad (15)$$

where the operators $\hat{\varepsilon}$ and $\hat{\eta}$ are the perturbation and then, assumed with small eigenvalues. Moreover, consider the well known perturbative expansion ⁽¹⁹⁾

$$\sin(\hat{\phi} + \hat{\varepsilon}) = \sin(\hat{\phi}) + Re \left(e^{i\hat{\phi}} \int_0^1 d\theta e^{-i\hat{\phi}\theta} \hat{\varepsilon} e^{i\hat{\phi}\theta} \right). \quad (16)$$

Since $\hat{\phi} = f\hat{P}_0$, and as said \hat{P}_0 is a projector, then from the above equation (and (3-4)) we have the linear evolution equation for the perturbation $\hat{\varepsilon}$:

$$LC \frac{\partial^2}{\partial t^2} \hat{\varepsilon} = Re \frac{\partial^2}{\partial x^2} \left(e^{i\frac{qf}{\hbar} \hat{P}_0} \int_0^1 d\theta e^{-i\frac{qf}{\hbar} \hat{P}_0 \theta} \hat{\varepsilon} e^{+i\frac{qf}{\hbar} \hat{P}_0 \theta} \right). \quad (17)$$

We shall consider two cases:

- (a) $\hat{\varepsilon} = \varepsilon(x, t) \hat{P}_0$. Here $[\hat{\varepsilon}, \hat{P}_0] = 0$ and then we have the linear wave equation $LC \frac{\partial^2}{\partial t^2} \varepsilon = \left(\cos \frac{qf}{\hbar} \right) \frac{\partial^2}{\partial x^2} \varepsilon$ and the perturbations are unstable when $\left(\cos \frac{qf}{\hbar} \right) < 0$.
- (b) $\hat{\varepsilon} = \varepsilon(x, t) (\hat{I} - \hat{P}_0)$. In this case the wave equation becomes $LC \frac{\partial^2}{\partial t^2} \varepsilon = \frac{\partial^2}{\partial x^2} \varepsilon$, and the perturbation is stable.

V. DUAL TRANSMISSION LINE

It is well known that the direct classical L-C transmission line (related to equation 1) has associated a dual transmission line: in the direct line the interaction between cells is through capacitances, while in the dual it is through inductances. The dual line is closely related to the so-called *left-handed* materials, and then its quantization is actually important. Moreover, the role of charge discreteness must be also considered. This two step process (quantization and charge discreteness) could be realized in analogy with the direct line (section I) but in this case long range interactions between cells appear in the Hamiltonian. In fact, the expression for the Hamiltonian is ⁽¹⁸⁾:

$$\hat{H} = \frac{\hbar^2}{2\pi L q_e^2} \sum_{l,n} \left(\int dk \frac{e^{ik(l-n)}}{1 - \cos k} \sin \frac{q_e}{2\hbar} \hat{\phi}_l \sin \frac{q_e}{2\hbar} \hat{\phi}_l \right) + \sum_l \frac{\hat{Q}_l^2}{2C}. \quad (18)$$

The equation of motion the charge and pseudoflux may be obtained after some algebra. We shall not continue the description of the dual line, but we shall only mention here that the expressions are quite involved and, so far, no explicit solution have been found.

VI. TODA LATTICE AND CIRQUITONS

The cirquiton Hamiltonian (1) gives the equations of motion for charge and pseudo-flux in the cell l :

$$\frac{\partial}{\partial t} \hat{\phi}_l = \frac{1}{C} \left(\hat{Q}_{l+1} + \hat{Q}_{l-1} - 2\hat{Q}_l \right), \quad (19)$$

$$\frac{\partial}{\partial t} \hat{Q}_l = \frac{\hbar}{Lq_e} \sin \frac{q_e}{\hbar} \hat{\phi}_l. \quad (20)$$

Equations (3-4) in section I are the spatially continuous version of the above pair of equations. Then, for the pseudo-flux operator we have the closed non linear equation of motion:

$$LC \frac{\partial^2}{\partial t^2} \hat{\phi}_l = \frac{\hbar}{q_e} \left(\sin \frac{q_e}{\hbar} \hat{\phi}_{l+1} + \sin \frac{q_e}{\hbar} \hat{\phi}_{l-1} - 2 \sin \frac{q_e}{\hbar} \hat{\phi}_l \right), \quad (21)$$

which, in the formal limit $q_e \rightarrow 0$ gives the usual one-band system with frequency spectrum $\omega(k) = \frac{2}{\sqrt{LC}} |\sin(k/2)|$, as expected. Consider now the equation:

$$LC \frac{\partial^2}{\partial t^2} \hat{\phi}_l = \frac{\hbar}{iq_e} \left(e^{\frac{iq_e}{\hbar} \hat{\phi}_{l+1}} + e^{\frac{iq_e}{\hbar} \hat{\phi}_{l-1}} - 2e^{\frac{iq_e}{\hbar} \hat{\phi}_l} \right), \quad (22)$$

then any hermitian solution of this last equation is also solution of the cirquiton equation (21). To show this, it suffices to conjugate Eq. (22) and subtracting. Notice that any hermitian solution of Eq.(22) is also a solution of (21), but the inverse is not necessarily true.

On the other hand, the broad field related to the Toda lattice is studied in depth in a variety of branches in physics¹⁷ including non-linear physics, statistical mechanics, classical electric circuits, etc. The classical evolution equation for the Toda lattice has the generic form:

$$M \frac{\partial^2}{\partial t^2} \phi_l = -A \left(e^{-B\phi_{l+1}} + e^{-B\phi_{l-1}} - 2e^{-B\phi_l} \right) \quad (23)$$

where M, A and B are real constant. So, we have the important result: the formal replacement $q_e \rightarrow iq_e$ transforms (22) into the (quantum) Toda lattice equation. This makes a direct connection between Toda lattice and cirquiton theory.

VII. FINAL REMARKS

For the quantum electric transmission line with charge discreteness described by the Hamiltonian Eq.(1), and equations of motion (3-4), a one parameter (f) wavefront solution was found (Eqs. 11-12). The condition Eq.(11) on the velocity generates a band-gap structure dependent on the pseudoflux parameter f (see figure 1), namely, there exist regions (values of f) for which a solitary wavefront propagates with constant speed. The existence of the band-gap structure described is the main result of this work.

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